Environment-induced anisotropy and the sensitivity of the radical pair mechanism in the avian compass

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Earth's magnetic field is essential for orientation in birds migration[1–6]. The most promising explanation for this orientation is the photo-stimulated radical pair (RP) mechanism [7–11], conjectured to occur in cryptochrome photoreceptors [12, 13]. The radicals must have an intrinsic anisotropy in order to define a reference frame for the compass [14–16]. This anisotropy, when introduced through hyperfine interactions, imposes immobility of the RP, and implies that entanglement between the unpaired electrons of the RP is preserved over long coherence times [17, 18]. We show that this kind of anisotropy, and consequently the entanglement in the model, are not necessary for the proper functioning of the compass. Classically correlated initial conditions for the RP, subjected to a fast decoherence process, are able to provide the anisotropy required. The environment in which the RP is immersed is then responsible for the reference frame of the compass, relaxing the immobility assumption. This fact significantly expands the range of applicability of the RP mechanism providing more elements for experimental search.

The ability of birds to use the Earth's magnetic field to orientate themselves in the correct direction for migration [1, 2] has originated several experimental works devoted to the understanding of the main features of the underlying mechanism [3–6]. One of the first proposals for modeling the appearance of the magnetic compass was that magneto-perception operates by means of anisotropic magnetic field effects on the rate of production of yields of a photostimulated radical pair reaction [14–16]. Although other models have been proposed, such as a magnetite-based magneto-perception [19, 20], the proposal of a radical pair mechanism (RPM) has been recently reinforced [7] and strong experimental evidences have been presented in its favor [8–10, 21, 22]. The solid state RPM model can be summarized as follows [7]: a molecular precursor reacts to form a pair of radicals due to photochemically-driven electron transfer. Taking into account that both radicals are created in a single event, it is natural to assume that the electron spins are initially entangled (in the following we assume that the radical pair (RP) is created in a singlet s state, although working with a triplet t state is also possible). This singlet state evolves under the influence of a Hamiltonian containing an hyperfine interaction term between the nuclei and their electrons and a Zeeman interaction term between the unpaired electrons. Due to the anisotropy of the hyperfine tensor, the interconversion between entangled singlet and triplet states depends on the direction of the applied magnetic field through the Zeeman term in the hamiltonian. It is necessary also to assume that the radicals are almost immobile, without significant diffusive motion, in order to avoid the anisotropy present in the system to be averaged away (Fig. 1 (a)). The RP yields depend on the relative alignment of the magnetic field in relation to the sample [23, 24], so that it can work as a compass.

In this work, we show that the anisotropy in the molecule can be replaced by an anisotropic environment (Figure 1(b)). This fact allows for a free isotropic molecule in a diffusive environment to work as a compass. In addition, although some discussion have been given recently about the importance of entanglement in the magneto-perception process [17, 18], this still remains obscure. In this sense, we also find that entanglement is neither necessary in our model of isotropic molecules nor in the anisotropic ones. Furthermore, we also verify the functioning of the compass in the presence of artificial radio frequency fields. We find that the isotropic model cannot work in the presence of such field in agreement with experimental findings [21, 25, 26]. However, the anisotropic model can work under some environmental conditions not unlikely in an open system, which notwithstanding disagree with experimental observation. This fact gives one more evidence in favor of the present model of an isotropic molecule.

Let us consider the Hamiltonian of the RP, neglecting all the other interactions, such as exchange and dipolar, to be:

$$\hat{H}^k = \sum_i \hat{\mathbf{I}}_{ik} \cdot A_{ik} \cdot \hat{\mathbf{S}}_k + \frac{g_e \mu_B}{\hbar} \mathbf{B} \cdot \hat{\mathbf{S}}_k, \tag{1}$$

where the first term is the hyperfine contribution and the second one is the Zeeman contribution, with i labeling the i-th nucleus in the k-th radical. Earth's magnetic field is given by $\mathbf{B} = B_0(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, and A is the hyperfine tensor. $\hat{\mathbf{I}}$ and $\hat{\mathbf{S}}$ are the spin operators for the nucleus and the electron respectively, g_e is the electron g-factor, $B_0 = 47\mu T$ and μ_B is the Bohr Magneton. We assume that the electron g_e-tensor is isotropic and close to that of a free electron, and that the hyperfine tensor A is, for simplicity, diagonal. Additionally, it can be either isotropic or anisotropic according to the model. The direction of the applied magnetic field in

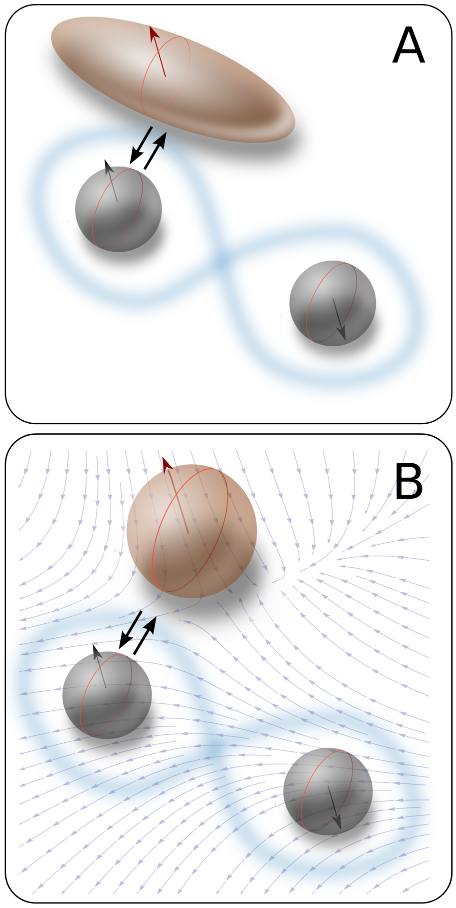

FIG. 1. Difference between the anisotropic RPM and the isotropic RPM with anisotropic environment.

relation to the RP fixed axis system is defined in terms of the polar angles (θ, ϕ); without losing generality we are going to assume $\phi = 0$ in order to simplify procedures. The most appropriate units to work with are those of Nuclear Magnetic Resonance (angular frequency units).

In order to fully determine the dynamics of our system, we are going to use a master equation approach [17]. To account for the singlet or the triplet yields, we add their formation rate to the master equation as a dissipative process modulated by a factor k in angular frequency units. The simplest model we can consider is one nucleus coupled with its unpaired electron plus a free electron. The evolution of the system can be written as

$$\begin{aligned}\frac{d}{dt}\rho(t) &= i\big[\rho(t), \hat{H}\big]/\hbar \\ &+ \sum_n \frac{k}{2}\big(2P_n\rho(t)P_n - P_n\rho(t) - \rho(t)P_n\big) \\ &+ \frac{P}{2}\big(2\hat{B}^\dagger\rho(t)\hat{B} - \hat{B}\hat{B}^\dagger\rho(t) - \rho(t)\hat{B}\hat{B}^\dagger\big) \\ &+ \frac{\gamma}{2}\big(2\hat{B}\rho(t)\hat{B}^\dagger - \hat{B}^\dagger\hat{B}\rho(t) - \rho(t)\hat{B}^\dagger\hat{B}\big).\end{aligned} \tag{2}$$

The operators P_n are projectors over the singlet or triplet shells as described in [17], and the sum is over all the different possible states (singlet for electronic states with nuclear spin up, i.e., $|s, 0, \uparrow\rangle$; triplet state with nuclear spin down, i.e., $|t, 0, \downarrow\rangle$, and so on); n runs in the nuclear and electronic spin states. The process mediated by k can be thought as a measurement on the state of the RP, giving us information about the amount of singlet or triplet yield. However the density operator formalism enable us to take into account the environment in which it lives. A wide range of noise processes are tested to model environmental interaction which result in decoherence times of hundreds of microseconds [17]. This conclusion was in agreement with the experimental results that show an interruption of the sensitivity when a *rf* field is applied. However, it seems natural to have a faster decoherence, if we take into account the very likely wildness of the environment surrounding the RP; we can accomplish this by choosing a suitable noise processes given by the operator $\hat{B}$. We define it as $\hat{B} = \hat{S}_{+1}\hat{S}_{-2}$, where $\hat{S}_{\pm,\{1,2\}}$ are the ladder operators for spins 1 and 2 respectively. The role of this operator is to flip spins $|\beta\alpha\rangle \leftrightarrow |\alpha\beta\rangle$, leaving the states $|\alpha\alpha\rangle$ and $|\beta\beta\rangle$ unchanged, thus intensifying the interconversion between singlet and triplet states, and introducing an environment-induced asymmetry. We add this interactions as Lindblad-like superoperators mediated by rates P and γ.

The yields *measurement* process, regardless of its magnitude, is not going to affect the performance of the compass. Therefore k could be arbitrarily high and the compass would still work. However, an upper bound to k is necessary and it can be determined by an important experimental observation: It was observed, in a set of experiments with European Robins, that an oscillating *rf* magnetic field $\vec{B}_{rf}$, perpendicular to the Earth's one, disrupts the avian compass functioning [21, 25], leaving them without sense of direction. So when the magnitude of k exceeds a threshold, the influence of the measurement process should overwhelm the action of the *rf* field [17], and as a result, the sensitivity to the variations of the magnetic field of Earth would be present despite of the disrupting effect. This fact can be contrasted to the experimental results to pick a suitable upper bound to k as $k = 0.01$MHz, which will be used unless stated otherwise. The processes mediated by P and γ show the same behavior, i.e., their influence will allow the compass to work in spite of the presence of the *rf* field if their magnitudes are high enough. As the experimental observation tell us that there will not be a compass if the birds are subject to this *rf* field, we use this to set upper bounds for the noise amplitudes. This fact also implies a lower limit for the decoherence time of the system, because an upper bound to the noise amplitudes implies that this time cannot be arbitrarily small, and we are going to have at least tens of microseconds until the loss of all coherences in the system. We use a magnitude $B_{rf} = 150$nT as proposed in those works.

As stated by Schulten [14], in order to the compass to work some kind of anisotropy must be present in the system. If, as usual, we choose the source of anisotropy in the hyperfine tensor, there is a sensitivity in the RPM to all initial states. To show that, we start by observing that for some values of the rates, for example $P = \gamma = 2k$, the influence of the rf field over the compass is strengthened; and if both P and γ are of

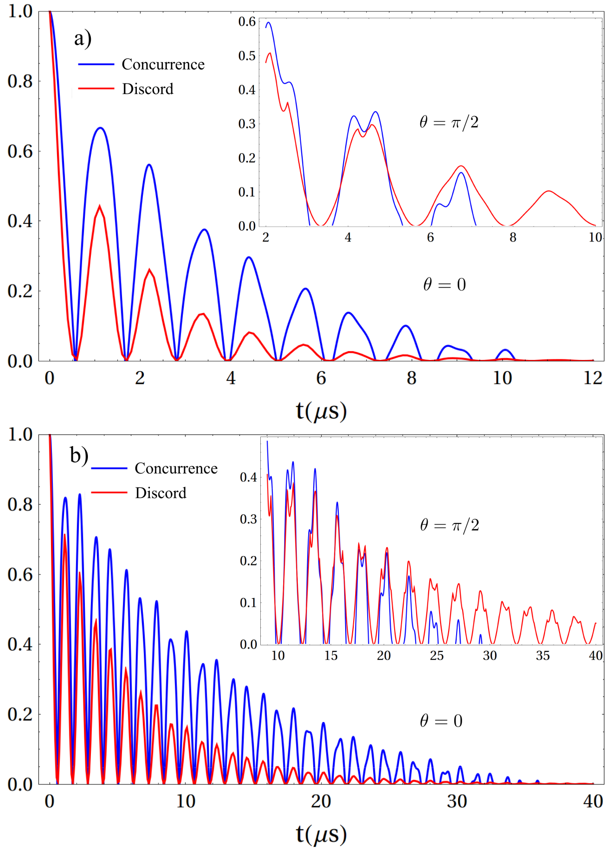

FIG. 2. Concurrence an Quantum Discord evolution for different values of the rates and magnetic field inclination angles. a) Measurement rate $k = 0.1MHz$, and dissipation rates $P = \gamma = 2k$, with and angle $\theta = 0$; in the inset an angle of $\theta = \pi/2$ was used. b) Measurement rate $k = 0.01MHz$, and dissipation rates $P = 10k$, $\gamma = 2k$, with and angle $\theta = 0$; in the inset an angle of $\theta = \pi/2$ was used. Is worth to note that the angle affect the amount of quantum correlations measured by the QD and the Concurrence; for smaller angles the Concurrence values are not only higher, but predict the same time of decoherence as the QD; however, for higher angles, the entanglement is less important than the classical correlations, making the QD to be higher and to predict longer correlation times.

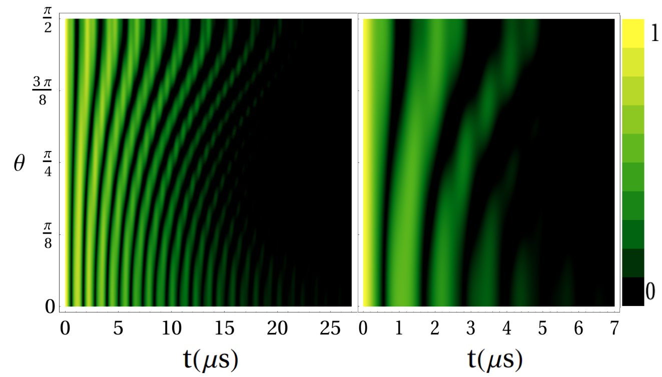

FIG. 3. Entanglement density for different values of the rates P, γ and k, varying the angles θ of inclination of the magnetic field of Earth ($47\mu T$). The entanglement was measured by the use of Concurrence. In the left panel, the rate values are $k = 0.01MHz$, $P = \gamma = 10k$, and in the right panel the values are $k = 0.05MHz$, $P = 10k$, $\gamma = 5k$. It's interesting to note that with smaller angles there are more entanglement sudden deaths and revivals, and that for angles around $\pi/4$ the decoherence time is shorter.

the order of $20k$ the compass-disrupting effect by the rf field can still be observed. It is interesting to note that even if in this situation the environment contributes to the insensitivity of the compass by means of the rf field, in other circumstances it can increase the sensitivity [27]. Also the presence of a gradient field was proven to increase the compass sensitivity [28]. One of the consequences of using the present process is that the decoherence times are short. To give a measure of those times for testing the model with anisotropy in the hyperfine tensor we use the Quantum Discord (QD) [29], which is able to take into account a more general kind of quantum correlations, and the Concurrence [30], which measures the amount of entanglement; the former is defined as

$$\delta_{\overleftarrow{AB}} = I_{AB} - J_{\overleftarrow{AB}},$$

where I_{AB} is the mutual information between A and B and is defined as $I_{AB} = S_A + S_B - S_{AB}$, S_x is the von Neumann entropy of system x, $J_{\overleftarrow{AB}} = \max_{\{\Pi_x^B\}}\left[S(\rho_A) - \sum_x p_x S(\rho_A^x)\right]$ is the classical correlation between the subsystems, $p_x = Tr_A\{\Pi_x^B \rho_{AB} \Pi_x^B\}$ and $\rho_A^x = Tr_B\{\Pi_x^B \rho_{AB} \Pi_x^B\}/p_x$; the maximum is taken over the positive measurements $\{\Pi_x^B\}$ made over the system B. The evolution of both, Quantum Discord and Concurrence can be seen in Figure (2). The fast loss of coherence is not a surprise - having an open environment like the one we can expect in the eye of the bird, should lead naturally to a fast loss of quantum correlations. This result should not compromise the correct behavior of the compass; one of the reasons, concerning the role of entanglement in the system, will be presented below. It is also interesting to note that the change in the inclination of the magnetic field also affects the loss of coherence. This can be seen in Figure (3), where the change of concurrence with time and inclination angle, for P and γ fixed, is shown. For small angles θ there are going to be more collapses and revivals of entanglement, and for angles near $\pi/4$, the decoherence time are shorter that for angles near 0 and $\pi/2$.

Following the discussion in Ref. [18], the initial state in the RPM is not a perfect singlet (or triplet) state, so a natural way to test if the quantum correlations play a fundamental role in the working of the compass is to choose non-entangled initial conditions. In [18] several random initial conditions were used, and the conclusion was that there is not a crucial dependence on the entanglement of the initial state, and that even RPs with initial separable states with only *classical correlations* can produce an inclination sensitivity in the singlet yield. We tested several random initial conditions, some of them entangled, with the hyperfine tensor in eq. (1) anisotropic, and with the decoherence processes turned off, i.e., $P = \gamma = 0$. The results show that the amount of entanglement is not a fundamental factor for the sensitivity in the change of the angle

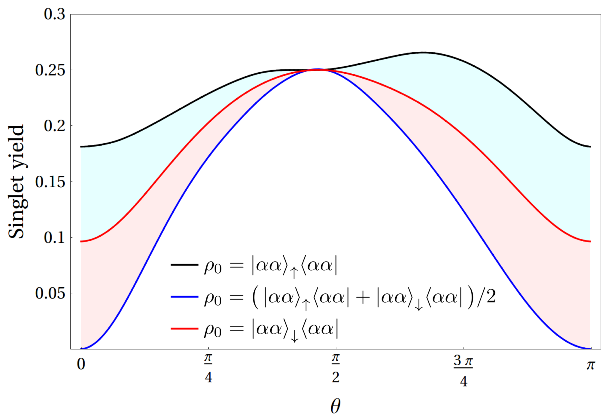

FIG. 4. Angle sensitivity for non singlet or triplet initial conditions, specifically $\rho_0 = |\alpha\alpha\rangle\langle\alpha\alpha|$. Black: nuclear spin initially set to $|\uparrow\rangle$. Blue: nuclear spin initially set to a mixed state $\big(|\uparrow\rangle+|\downarrow\rangle\big)/\sqrt{2}$. Red: nuclear spin initially set to $|\downarrow\rangle$.

of the applied magnetic field. As an example, an initial state

$$\rho_0 = \frac{1}{2}\big(|\alpha\beta\rangle\langle\alpha\beta| + |\beta\alpha\rangle\langle\beta\alpha|\big), \tag{3}$$

gives an appreciable change in the yields (and therefore allow sensitivity) for different angles θ.

However, we found two cases in which *without explicit anisotropy* in the hamiltonian (1) there is still a fully functional compass. The first one, with $P = \gamma = 0$, is due to the initial condition: if it is not an entangled one the system is still sensitive to changes in the inclination of the field. In other words, in the absence of an explicit anisotropy in the hyperfine tensor or in the g electronic factor, the sensitivity depends on the *inhomogeneity* of the populations in the density matrix. As an example consider a state like eq. (3), i.e., without coherences: Its yield distribution, the blue curve in the Figure (4), shows a high variation with the angle. Moreover, an initial state like $\rho_0 = |\alpha\alpha\rangle\langle\alpha\alpha|$, which produces a lower but still appreciable angle sensitivity, generates a different distribution for the singlet yield depending on the nuclear spin state, as is shown in Figure (4), exemplifying the reach and relevance of this source of anisotropy. Now we check the anisotropy introduced by the environment - when there is a fast enough decoherence process present in the master equation, like the processes mediated by P and γ introduced before. If the hamiltonian is isotropic, with singlet or triplet initial conditions, the expected behavior is an absence of change in the production rates of the yields, and there is going to be sensitivity only if there is a decoherence process present. This can be understood as another class of anisotropy induced by the environment, which chooses a preferred direction for the system through the dissipation. This can open the search of a suitable chemical species responsible for the RP creation, because the molecule does not need to present anisotropic hyperfine or Zeeman interactions, and the degree of entanglement is not going to be crucial. The only requirement for the correct functionality of the compass is then the decoherence, which is a must in such an open system. Both cases can be seen in Figure (5).

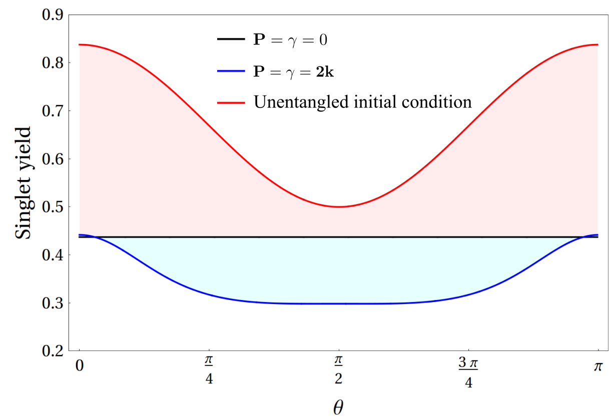

FIG. 5. Angle sensitivity of isotropic hamiltonians with $k = 0.01$. Black: evolution of the singlet yield for different angles with an entangled initial condition. Blue: evolution of the singlet yield for different angles with an entangled initial condition and $P = \gamma = 2k$. Red: Evolution of the singlet yield for different angles with an unentangled initial condition.

Our findings go beyond establishing the role of the entanglement in the compass. We found that any kind of correlation, quantum or classical, is sufficient for the RPM if the molecule is anisotropic, and that an isotropic molecule can have sensitivity for variations in the field *even* if it has classically correlated, separable initial conditions. One example of such a state is given by eq. (3). Furthermore, even if they lack any kind of correlation but are *anisotropic*, giving an unbalanced weight to some populations over others, like the states used in Figure (4), we can also expect a working compass. A careful analysis has to be made in order to transparently identify the characteristics of the initial conditions that lead to a dependence of the singlet yield with the inclination angle of the field.

As discussed in [23, 24], the anisotropy of a molecule can be averaged away if it has significant diffusive motion, or even rotations. Our findings of unexpected sources of anisotropy relax this immobility requirement. This is highly positive for the model given the wild conditions involving actual bio-photochemical processes. Along with this, isotropic molecules seem to be more robust to environmental effects; in the presence of a rf field the control experimental data[21, 25] shows that the compass will no longer work. However, if there is a strong enough dissipation the compass will work normally[17]. An isotropic molecule can handle higher noise magnitudes than an anisotropic one without jeopardizing control experimental data.

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